

5,6-Dimethylbenzimidazole

Inchi:	InChI=1S/C9H10N2/c1-6-3-8-9(4-7(6)2)11-5-10-8/h3-5H,1-2H3,(H,10,11)
InchiKey:	LJUQGASMPRMWIW-UHFFFAOYSA-N
Formula:	C9H10N2
SMILES:	Cc1cc2nc[nH]c2cc1C
Mol. weight [g/mol]:	146.19
CAS:	582-60-5

Physical Properties

Property code	Value	Unit	Source
hf	117.28	kJ/mol	Cheméo Relay (1.0)
ie	8.03	eV	Cheméo Relay (1.0)
logp	1.698		Crippen Method
mcvol	118.710	ml/mol	McGowan Method
tf	478.65	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

Legend

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

tf: Normal melting (fusion) point

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